

Cumene

98-82-8 | DTXSID1021827

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 3.77

Global applicability domain: Inside

Local applicability domain index: 6.40e-01

Confidence level: 6.67e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Cumene

Measured: 3.66

Predicted: 3.77

[Image not found](#)

1-Ethyl-2-methylbenzene

Measured: 3.53

Predicted: 3.47

[Image not found](#)

3-fluoropropylbenzene

Measured: 2.95

Predicted: 3.43

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p-Propyltoluene

Measured: 4.60

Predicted: 4.29